

AMENDMENTS TO THE CLAIMS

1. (Currently Amended) A system for improved modeling of a biological system that comprises a plurality of chemical reactions, the system comprising:

a modeling component ~~comprising~~ having a graphical user interface for accepting user commands and input to construct or modify a model of the biological system;

a simulation engine conducting a simulation of the model by accepting as input the ~~constructed~~ model of the biological system and generating as output dynamic behavior of the biological system until the occurrence of a predefined simulation termination condition; and

an analysis environment in communication with the simulation engine, the analysis environment

interfacing with data acquisition hardware that gathers data from an experiment,
and

using the output of the simulation engine to control a property of the experiment,
the output representing the dynamic behavior of the biological system at a completion of the simulation.

2. (Original) The system of claim 1 wherein the modeling component allows construction of a block diagram model of the biological system.

3. (Original) The system of claim 2 wherein the modeling component further includes at least one block identifying a set of related chemical reactions.

4. (Original) The system of claim 1 wherein the modeling component includes a tool palette for aiding construction of the model of the biological system.

5. (Previously Presented) The system of claim 1 wherein the simulation engine generates the dynamic behavior of the biological system using a stochastic computational model.

6. (Withdrawn) The system of claim 1 wherein said simulation engine generates the dynamic behavior of the biological system using a discrete time-based computational model.

7. (Withdrawn) The system of claim 1 wherein said simulation engine generates the dynamic behavior of the biological system using a continuous time-based computational model.

8. (Currently Amended) A computer-implemented improved method for modeling a biological process comprising a plurality of chemical reactions, the method comprising:

~~providing a graphical user interface;~~

~~—receiving, via the provided user interface, user commands and data;~~

~~—constructing, using the received user commands and data, a model of the biological process;~~

~~generating, using the constructed~~performing a simulation of a model of the a biological process, dynamic behavior of the modeled biological process until the occurrence of a predefined simulation termination condition to generate dynamic behavior of the modeled biological process; and

providing an indication that data gathered ~~from~~at the conclusion of an experiment and the generated dynamic behavior at a completion of the simulation differ by an amount greater than a predetermined amount, if a difference between the data gathered from the experiment and the generated dynamic behavior is greater than the predetermined amount.

9. (Previously Presented) The method of claim 8 wherein constructing further comprises:

constructing a block diagram model of the biological process.

10. (Original) The method of claim 9 wherein the block diagram model includes at least one block identifying a set of related chemical reactions.

11. (Previously Presented) The method of claim 8 wherein generating further comprises:

generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process using a stochastic computational model.

12. (Withdrawn) The method of claim 8 wherein generating further comprises:

generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process using a discrete time-based computational model.

13. (Withdrawn) The method of claim 8 wherein generating further comprises:

generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process using a continuous time-based computational model.

14. (Currently Amended) An article of manufacture having embodied thereon computer-readable instructions for improved modeling of a biological process comprising a plurality of chemical reactions, the article of manufacture comprising:

~~computer readable instructions for providing a graphical user interface;~~
~~computer readable instructions for receiving, via the provided user interface, user commands and data;~~
~~computer readable instructions for constructing, using the received user commands and data, a model of the biological process;~~
computer-readable instructions for ~~generating, using the constructed~~performing a simulation of a model of ~~the a~~ biological process, ~~dynamic behavior of the modeled biological process~~ until the occurrence of a predefined simulation termination condition to generate dynamic behavior of the modeled biological process; and
computer-readable instructions for providing an indication that data gathered ~~from~~ at a conclusion of an experiment and the generated dynamic behavior at a completion of the simulation differ by an amount greater than a predetermined amount, if a difference between the data gathered from the experiment and the generated dynamic behavior is greater than the predetermined amount.

15. (Previously Presented) The article of manufacture of claim 14 wherein the computer-readable instructions for constructing a model of the biological process comprises computer-readable instructions for constructing a block diagram model of a biological process.

16. (Previously Presented) The article of manufacture of claim 15 wherein the computer-readable instructions for constructing a block diagram model of the biological process includes computer-readable instructions for constructing at least one block identifying a set of related chemical reactions.

17. (Previously Presented) The article of manufacture of claim 14 wherein the computer-readable instructions for generating dynamic behavior of the modeled biological process comprises computer-readable instructions for generating dynamic behavior of the modeled biological process using a stochastic computational model.

18. (Withdrawn) The article of manufacture of claim 14 wherein computer-readable instructions for generating dynamic behavior of the modeled biological process comprises computer-readable instructions for generating dynamic behavior of the modeled biological process using an event-based computational model.

19. (Withdrawn) The article of manufacture of claim 14 wherein computer-readable instructions for generating dynamic behavior of the modeled biological process comprises computer-readable instructions for generating dynamic behavior of the modeled biological process using a continuous time-based computational model.

20. (Currently Amended) A system for improved modeling of a chemical reaction comprising:
a modeling environment accepting user commands and input for constructing a model of a chemical reaction;

a simulation engine conducting a simulation of the model by accepting as input the constructed model of the chemical reaction and generating as output an expected result upon the occurrence of a predefined simulation termination condition; and

an analysis environment in communication with the simulation engine, the analysis environment

interfacing with data acquisition hardware that gathers data from an experiment,
and

using the output of the simulation engine to control a property of the experiment,
the output representing the expected result of the chemical reaction at a completion of the simulation.

21. (Original) The system of claim 20 wherein the modeling environment allows construction of a block diagram model of a chemical reaction.

22. (Original) The system of claim 21 wherein the modeling environment further includes at least one block identifying a set of related chemical reactions.

23. (Previously Presented) The system of claim 20 wherein the simulation engine generates an expected result using a stochastic computational model.

24. (Withdrawn) The system of claim 20 wherein said simulation engine generates an expected result using a discrete time-based computational model.

25. (Withdrawn) The system of claim 20 wherein said simulation engine generates an expected result using a continuous time-based computational model.

26. (Currently Amended) A computer-implemented method for integrated modeling, simulation and analysis of chemical reactions, the method comprising:

~~providing a graphical user interface for accepting user commands and data;~~
~~receiving, via the provided user interface, user commands and data;~~
~~constructing, using the received user commands and data, a model of a chemical reaction;~~

~~generating, using the constructed~~ performing a simulation of a model of the a chemical reaction, an expected result of the modeled chemical reaction in a simulation until the occurrence of a predefined simulation termination condition to generate an expected result of the modeled chemical reaction; and

providing an indication that data gathered ~~from~~ at a conclusion of an experiment and the generated expected result at a completion of the simulation differ by an amount greater than a predetermined amount, if a difference between the data gathered from the experiment and the generated expected result is greater than the predetermined amount.

27. (Previously Presented) The method of claim 26 wherein constructing further comprises:
constructing a block diagram model of a chemical reaction.

28. (Original) The method of claim 27 wherein the block diagram model includes at least one block identifying a set of related chemical reactions.

29. (Previously Presented) The method of claim 26 wherein generating further comprises:

generating, using the constructed model of the chemical reaction, an expected result of the modeled chemical reaction using a stochastic computational model.

30. (Withdrawn) The method of claim 26 wherein generating further comprises:

generating, using the constructed model of the chemical reaction, an expected result of the modeled chemical reaction using a discrete time-based computational model.

31. (Withdrawn) The method of claim 26 wherein generating further comprises:

generating, using the constructed model of the chemical reaction, an expected result of the modeled chemical reaction using a continuous time-based computational model.

32. (Currently Amended) An article of manufacture having embodied thereon computer-readable instructions for integrated modeling, simulation and analysis of chemical reactions, the article of manufacture comprising:

~~computer readable instructions for providing a graphical user interface for accepting user commands and data;~~

~~computer readable instructions for receiving, via the provided user interface, user commands and data;~~

~~computer readable instructions for constructing, using the received user commands and data, a model of a chemical reaction;~~

~~computer-readable instructions for generating, using the constructed performing a simulation of a model of the chemical reaction, an expected result of the modeled chemical reaction until the occurrence of a predefined simulation termination condition to generate an expected result of the modeled chemical reaction in a simulation;~~ and

~~computer-readable instructions for providing an indication that data gathered ~~from~~ at a conclusion of an experiment and the generated expected result at a completion of the simulation differ by an amount greater than a predetermined amount, if a difference between the data gathered from the experiment and the generated expected result is greater than the predetermined amount.~~

33. (Previously Presented) The article of manufacture of claim 32 wherein the computer-readable instructions for constructing a model of the chemical reaction comprises computer-readable instructions for constructing a block diagram model of a chemical reaction.

34. (Previously Presented) The article of manufacture of claim 33 wherein the computer-readable instructions for constructing a block diagram model of the chemical reaction includes computer-readable instructions for constructing at least one block identifying a set of related chemical reactions.

35. (Previously Presented) The article of manufacture of claim 32 wherein computer-readable instructions for generating an expected result of the modeled chemical reaction comprises computer-readable instructions for generating an expected result of the modeled chemical reaction using a stochastic computational model.

36. (Withdrawn) The article of manufacture of claim 32 wherein computer-readable instructions for generating an expected result of the modeled chemical reaction comprises computer-readable instructions for generating an expected result of the modeled chemical reaction using an event-based computational model.

37. (Previously Presented) The system of claim 1 wherein the tabular view and the graphical view of the model comprise annotations to the model that are provided by a user, the annotations being displayed in an annotation column of the tabular view and in a location close to an element of the model in the graphical view.

38. (Previously Presented) The method of claim 8 wherein the tabular view and the graphical view of the model comprise annotations to the model that are provided by a user, the annotations being displayed in an annotation column of the tabular view and in a location close to an element of the model in the graphical view.

39. (Previously Presented) The article of manufacture of claim 14 wherein the tabular view and the graphical view of the model comprise annotations to the model that are provided by a user,

the annotations being displayed in an annotation column of the tabular view and in a location close to an element of the model in the graphical view.